

A convenient method to prepare the effective pure state in a quantum ensemble

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Abstract

A simple method is proposed to prepare conveniently the effective pure state $|00\dots 0\rangle\langle 0\dots 00|$ with any number of qubits in a quantum ensemble. The preparation is based on the temporal averaging (Knill, Chuang, and Laflamme, Phys. Rev. A 57, 3348 (1998)). The quantum circuit to prepare the effective pure state is designed in a unified and systematical form and is explicitly decomposed completely into a product of a series of one-qubit quantum gates and the two-qubit diagonal quantum gates. The preparation could be programmed and implemented conveniently on an NMR quantum computer.

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1. Introduction

Quantum computers can solve certain problems that can not be solved by any classical digital computers [1-5]. Particularly, the prime factorization of a large number can be performed in a polynomial time on a quantum computer [3]. This has stimulated the experimental work of quantum computation in various physical disciplines including quantum optics [6], trapped ions [7], nuclear spin system [8], superconducting Josephson junctions [9], and so forth. Quantum computation is usually performed in a pure quantum state at any time [10]. However, recently it has been shown that quantum computation may be implemented in a spin quantum ensemble at a finite temperature by using nuclear magnetic resonance (NMR) techniques [11, 12]. After that, there has been a flood of experimental work of ensemble quantum computation on few-qubit systems [13-20]. The key of the approach is that a

quantum ensemble can be prepared in certain mixed states, i.e., the effective pure states [11] or the pseudopure states [12]. An effective pure state is a mixed state in a quantum ensemble that behaves for all computational purposes as a pure state, that is, the effective pure state is isomorphic to the pure state. Therefore, the reversible quantum computation can be performed in an effective pure state just like in a pure quantum state. The key step in the approach is then the preparation of the effective pure states. There are several methods to prepare the effective pure states or the pseudopure states. These include logical labeling [11, 21], spatial averaging [12, 22], temporal averaging [23], spectral labeling [17], and so forth. The temporal averaging method is really a technique much similar to the time averaging, coherent accumulation, and phase cycling techniques in NMR experiments [24, 25], but used for preparation of the effective pure states. This method has been investigated thoroughly by Knill, Chuang, and Laflamme [23]. The method such as the exhaustive averaging method usually involves cyclicly permuting the nonground states in $2^n - 1$ different ways such that the average of the prepared states is an effective pure state. Therefore, number of experiments to prepare the effective pure state grows exponentially as the qubit numbers n , showing that this method may be reasonable to consider implementing the preparation for small numbers of qubits. The advantage of the method over other preparations [11, 12] may be that it is a simple method to give a higher signal-to-noise ratio for the NMR experimental measurement.

In this paper a simple method is proposed to prepare conveniently the effective pure state $\rho_{eff} = \lambda|00...0\rangle\langle 0...00|$ in a spin quantum ensemble that consists of a large amount of two-state n -spin ($I=1/2$) quantum systems corresponding to the pure quantum ground state $|00...0\rangle$ of the quantum system. It is also based on the temporal averaging [23]. However, the preparation starts generally from the specific reduced density operator of the longitudinal n -spin order component $\sigma(0) = 2^{n-1}I_{1z}I_{2z}...I_{nz}$ [26, 27] that can be easily obtained from the equilibrium magnetization in the spin quantum ensemble (called also the spin system without confusion). The quantum circuit to prepare the effective pure state with any number of qubits is designed in a unified and systematical form. It is then explicitly decomposed completely into a product of a series of one-qubit quantum gates and the two-qubit diagonal gates [26]. Therefore, the preparation could be programmed and implemented conveniently on an NMR quantum computer.

2. Preparation of the effective pure states

An effective pure state or pseudopure state $\rho_{eff}(\Psi)$ in a quantum ensemble corresponding to the pure quantum state $|\Psi\rangle$ may be defined as [11, 12]

$$\rho_{eff}(\Psi) = (1 - \lambda)E + \lambda|\Psi\rangle\langle\Psi| \quad (1)$$

where the normalization factor is omitted without confusion, λ is a real constant, and E is $N (= 2^n)$ -dimensional unity operator. Because the unity operator is unobservable and keeps unchanged when it is acted on by an arbitrary unitary transformation the mixed state $\lambda|\Psi\rangle\langle\Psi|$ and the effective pure state $\rho_{eff}(\Psi)$ cannot be distinguished by standard NMR experiments. Therefore, the process of NMR ensemble quantum computing can be really characterized completely through the reduced effective pure state $\sigma_{eff} = \lambda|\Psi\rangle\langle\Psi|$. In order to make use of the massive quantum parallelism [2] the superposition in a quantum system is usually created at the first step in quantum computing, while the superposition in a spin quantum ensemble can be created conveniently by acting the Walsh-Hadamard transform W [5] on the effective pure state corresponding to the pure quantum groundstate $|00\dots 0\rangle$ in the quantum system:

$$\sigma_{eff} = \lambda|00\dots 0\rangle\langle 0\dots 00| \quad (2)$$

Thus, in the paper a simple method is proposed how to prepare conveniently the effective pure state of Eq.(2) in a spin quantum ensemble with any number of qubits.

First of all, the starting density operator $\rho(0)$ of the spin quantum ensemble is subjected to a unitary transformation whose unitary operator $\exp(-i\alpha Q)$ is constructed with the Hermitian operator Q defined by $Q_{ij} = 1$ for all indexes i and j :

$$\begin{aligned} \exp(-i\alpha Q)\rho(0)\exp(i\alpha Q) &= \rho(0) - \frac{1 - \cos(\alpha N)}{N}[\rho(0), Q]_+ \\ &+ i\frac{\sin(\alpha N)}{N}[\rho(0), Q]_- + \frac{[1 - \cos(\alpha N)]^2 + \sin^2(\alpha N)}{N^2}Q\rho(0)Q \end{aligned} \quad (3)$$

where $[\rho(0), Q]_{\pm} = \rho(0)Q \pm Q\rho(0)$ and the following expansion for the unitary operator $\exp(\pm i\alpha Q)$ has been introduced in the above transformation,

$$\exp(\pm i\alpha Q) = E - \frac{1 - \exp(\pm i\alpha N)}{N}Q \quad (4)$$

It follows from the definition of the operator Q , that is, $Q_{ij} = 1$ for all indexes i and j , that the product $Q\rho(0)Q$ can be reduced to the simple form

$$Q\rho(0)Q = Qf\{\rho(0)\} \quad (5)$$

where the function $f\{\rho(0)\}$ is defined as

$$f\{\rho(0)\} = \sum_{k,l=1}^N \rho_{kl}(0) \quad (6)$$

For convenience, one writes conveniently the density operator as the general form

$$\rho(0) = Tr\{E\}^{-1}E + \sigma(0), \quad (7)$$

where $\sigma(0)$ is the traceless reduced density operator, $Tr\{\sigma(0)\} = 0$. For an NMR spin quantum ensemble the high-temperature approximation holds and equation (7) is met. Obviously, it proves easily with the aid of Eq.(7) that equation (3) still holds when replacing the reduced density operator $\rho(0)$ with the density operator $\sigma(0)$. To simplify further Eq.(3) the operator Q is decomposed explicitly as

$$Q = N \exp(-i\frac{\pi}{2}F_y)D_0 \exp(i\frac{\pi}{2}F_y) \quad (8)$$

where the operator $F_\mu = \sum_{k=1}^n I_{k\mu}$, ($\mu = x, y, z$), $I_{k\mu} = \frac{1}{2}\sigma_{k\mu}$, σ is the Pauli's operator and the diagonal operator D_s is defined as

$$D_s = Diag[0, \dots, 0, 1, 0, \dots, 0], ([D_s]_{ss} = 1; [D_s]_{ii} = 0, i \neq s).$$

Then by exploiting Eqs.(5) and (8) one obtains from Eq.(3) that

$$\begin{aligned} & \frac{[1 - \cos(\alpha N)]^2 + \sin^2(\alpha N)}{N} f\{\rho(0)\} D_0 \\ &= \exp(-iN\alpha D_0) \rho_+(0) \exp(iN\alpha D_0) - \rho_+(0) \\ & \quad + (1 - \cos(\alpha N)) [\rho_+(0), D_0]_+ - i \sin(\alpha N) [\rho_+(0), D_0]_- \end{aligned} \quad (9)$$

where $\rho_+(0) = \exp(i\frac{\pi}{2}F_y)\rho(0)\exp(-i\frac{\pi}{2}F_y)$. In particular, if the parameter α in Eq.(3) is chosen suitably so that $\cos(\alpha N) = -1$ and $\sin(\alpha N) = 0$, then equation (9) can be further written as with the help of Eq.(7)

$$\begin{aligned} & \frac{4}{N} f\{\sigma(0)\} D_0 = \exp(-iN\alpha D_0) \sigma_+(0) \exp(iN\alpha D_0) \\ & \quad - \sigma_+(0) + 2[\sigma_+(0), D_0]_+ \end{aligned} \quad (10)$$

where $\sigma_+(0) = \exp(i\frac{\pi}{2}F_y)\sigma(0)\exp(-i\frac{\pi}{2}F_y)$. Now, the function $f\{\sigma(0)\} = 0$ if the density operator $\sigma(0)$ is taken as an arbitrary operator of the operator set $G = \{I_{ky}, I_{kz}, 2I_{ky}I_{lx}, 2I_{ky}I_{ly}, 2I_{ky}I_{lz}, 2I_{kz}I_{lx}, \dots\}$, which does not contain all the x-components and unity operator of the operator set $G_x = \{E, I_{kx}, 2I_{kx}I_{lx}, 4I_{kx}I_{lx}I_{mx}, \dots\}$. Then in this case equation (10) can be further simplified to the form

$$\begin{aligned} & \exp(-iN\alpha D_0) \sigma_+(0) \exp(iN\alpha D_0) - \sigma_+(0) \\ &= -2[\sigma_+(0), D_0]_+ \end{aligned} \quad (11)$$

When the starting density operator $\sigma(0)$ is taken as an arbitrary operator of set G_x equation (10) becomes an identity although in this case $f\{\sigma(0)\} \neq 0$. According to the definition of the diagonal operator D_0 and $\cos(\alpha N) = -1$, $\sin(\alpha N) = 0$ it turns out easily that

$$\exp(\pm iN\alpha D_0) = \text{Diag}[-1, 1, \dots, 1] = -R \quad (12)$$

where R is the phase-shift operation defined in the Grover quantum search algorithm [5]. By exploiting the definition of diffusion transform $D = WRW$ in the Grover quantum search algorithm [5], equation (11) is rewritten as

$$(2/N)[\sigma_+(0), ND_0]_+ = \sigma_+(0) - WDW\sigma_+(0)WDW \quad (13)$$

Equation (13) is the key to prepare conveniently the effective pure state $\rho_{eff} = \lambda|00\dots 0\rangle\langle 00\dots 0|$ in the paper.

It follows from the definition of the operator D_0 that the diagonal operator D_0 is really an effective pure state $\rho_{eff} = |00\dots 0\rangle\langle 0\dots 00| = D_0$. Because D_0 is a diagonal operator it can be expanded as a sum of the base operators of the longitudinal magnetization and spin order (*LOMSO*) operator subspace of the Liouville operator space of the n-spin ($I=1/2$) system [17, 26, 27]

$$ND_0 = E + \sum_{k=1}^n 2I_{kz} + \sum_{l>k=1}^n 4I_{kz}I_{lz} + \sum_{m>l>k=1}^n 8I_{kz}I_{lz}I_{mz} + \dots \quad (14a)$$

$$= (E_1 + 2I_{1z}) \otimes (E_2 + 2I_{2z}) \otimes \dots \otimes (E_n + 2I_{nz}) \quad (14b)$$

where E_k is 2×2 -dimensional unity operator of the k th qubit in the spin system. In order to extract the effective pure state from the term $[\sigma_+(0), ND_0]_+$ on the left-hand side of Eq.(13) the density operator $\sigma_+(0)$ needs to be chosen suitably. First, a series of the density operators $\sigma_+(0)$ are suitably chosen, where each density operator $\sigma(0)$ is only taken as an arbitrary operator of set G so that $f\{\sigma(0)\} = 0$ can be met, then the term $[\sigma_+(0), ND_0]_+$ is expanded explicitly by inserting each $\sigma_+(0)$ into the term. By exploiting these expansions one can construct explicitly the effective pure state $\rho_{eff} = \lambda|00\dots 0\rangle\langle 00\dots 0|$. The detailed procedure to prepare conveniently and explicitly the effective pure state based on equation (13) is illuminated below.

2.1 The logical labeling effective pure state

It has been shown that the following state, called the logical labeling effective pure state, can be thought of as an effective pure state if one of the qubits in the quantum system is used as a logical label [23]

$$\rho_{lb} = \delta E + \lambda(|00\dots 0\rangle\langle 0\dots 00| - |11\dots 1\rangle\langle 1\dots 11|). \quad (15)$$

It will be shown below that the logical labeling effective pure state of Eq.(15) in the n-spin system can be prepared on the basis of Eq.(13). The density operator $\sigma_+(0)$ in Eq.(13) is chosen simply as

$$\sigma_+(0) = 2^{n-1}I_{1y}I_{2y}\dots I_{ny} \quad (16)$$

Obviously, the function $f\{\sigma(0)\} = 0$. It is easy to turn out by using Eq.(14) that

$$[\sigma_+(0), ND_0]_+ = 2^{n-1}i^n I_1^- I_2^- \dots I_n^- + 2^{n-1}(-i)^n I_1^+ I_2^+ \dots I_n^+ \quad (17)$$

$$\begin{aligned}
&= 2^{n-1}(I_1^- I_2^- \dots I_n^- + I_1^+ I_2^+ \dots I_n^+), & \text{if } n = 4m \\
&= 2^{n-1}i(I_1^- I_2^- \dots I_n^- - I_1^+ I_2^+ \dots I_n^+), & \text{if } n = 4m + 1 \\
&= -2^{n-1}(I_1^- I_2^- \dots I_n^- + I_1^+ I_2^+ \dots I_n^+), & \text{if } n = 4m + 2 \\
&= -2^{n-1}i(I_1^- I_2^- \dots I_n^- - I_1^+ I_2^+ \dots I_n^+), & \text{if } n = 4m + 3.
\end{aligned}$$

The right-hand side of Eq.(17) is actually an n -qubit maximum entanglement state of the system. Therefore, one can prepare conveniently the maximum entanglement state through Eq.(13). Now, if n is an even number one makes a unitary transformation on the term $[\sigma_+(0), ND_0]_+$ to convert it into the form corresponding to n being an odd number

$$\begin{aligned}
&\exp(-i\theta F_z)(I_1^- I_2^- \dots I_n^- + I_1^+ I_2^+ \dots I_n^+) \exp(i\theta F_z) = \\
&\quad i(I_1^- I_2^- \dots I_n^- - I_1^+ I_2^+ \dots I_n^+)
\end{aligned}$$

where $n\theta = \pi/2$, that is, $\exp(\pm i n\theta) = \pm i$. Therefore, no matter that n is either an odd number or an even number one can prepare further the effective pure state by starting from the n -order multiple-quantum coherence $2^{n-1}i(I_1^- I_2^- \dots I_n^- - I_1^+ I_2^+ \dots I_n^+)$. By making a unitary transformation on the multiple-quantum coherence one obtains the logical labeling effective pure state of Eq.(15) without the unity operator term

$$\begin{aligned}
&\exp(-i\frac{\pi}{4} \times 2^n I_{1x} I_{2x} \dots I_{nx}) 2^{n-1}i(I_1^- I_2^- \dots I_n^- - I_1^+ I_2^+ \dots I_n^+) \\
&\times \exp(i\frac{\pi}{4} \times 2^n I_{1x} I_{2x} \dots I_{nx}) \\
&= \frac{1}{2}N(|00\dots 0\rangle\langle 0\dots 00| - |11\dots 1\rangle\langle 1\dots 11|)
\end{aligned} \tag{18}$$

On the other hand, by using Eq.(13) one can design the quantum circuit to prepare conveniently the logical labeling effective pure state of Eq.(18). As an example, consider the case of $n = 4m + 1$, by inserting Eq.(16) into Eq.(13) one obtains the logical labeling effective pure state of Eq.(18)

$$\begin{aligned}
\rho_{lb} &= (|00\dots 0\rangle\langle 0\dots 00| - |11\dots 1\rangle\langle 1\dots 11|) \\
&= 2^{n-1}I_{1z}I_{2z}\dots I_{nz} - \exp(-i\frac{\pi}{4} \times 2^n I_{1x}I_{2x}\dots I_{nx})WDW \exp(i\frac{\pi}{2}F_x) \\
&\quad \times 2^{n-1}I_{1z}I_{2z}\dots I_{nz} \exp(-i\frac{\pi}{2}F_x)WDW \exp(i\frac{\pi}{4} \times 2^n I_{1x}I_{2x}\dots I_{nx})
\end{aligned} \tag{19}$$

Experimentally, starting from the reduced density operator, i.e., the longitudinal n -spin order component $\sigma(0) = 2^{n-1}I_{1z}I_{2z}\dots I_{nz}$ that can be prepared from the thermal equilibrium state in an n -spin quantum ensemble one performs two different experiments to prepare the logical labeling effective pure state ρ_{lb} of Eq.(18) according to Eq.(19), one experiment with the identical operation E and another with the unitary operation $\exp(-i\frac{\pi}{4} \times 2^n I_{1x}I_{2x}\dots I_{nx})WDW \exp(i\frac{\pi}{2}F_x)$. In comparison with the flip and swap method [23] to prepare the logical labeling effective pure state of Eq.(15) the present method is still available even when the number of qubits (n) and the polarization (δ) of the quantum system satisfy $n\delta \sim 1$ or when the initial state of the system does not have approximate inversion symmetry, but as shown in

Ref.[23], in these cases the flip and swap method is failure.

2.2 The effective pure states

(a) A two-spin system

The density operator $\sigma_+(0)$ is chosen as $\sigma_+(0) = 2I_{1y}I_{2z}, 2I_{1z}I_{2y}$, respectively. One obtains with the help of Eq.(14)

$$\begin{aligned} & \exp(-i\frac{\pi}{2}I_{1x})[2I_{1y}I_{2z}, ND_0]_+ \exp(i\frac{\pi}{2}I_{1x}) \\ &= \frac{1}{2}ND_0 - \frac{1}{2}(E_1 - 2I_{1z}) \otimes (E_2 + 2I_{2z}), \end{aligned} \quad (20a)$$

$$\begin{aligned} & \exp(-i\frac{\pi}{2}I_{2x})[2I_{1z}I_{2y}, ND_0]_+ \exp(i\frac{\pi}{2}I_{2x}) \\ &= \frac{1}{2}ND_0 - \frac{1}{2}(E_1 + 2I_{1z}) \otimes (E_2 - 2I_{2z}) \end{aligned} \quad (20b)$$

By plus Eqs.(20a) and (20b) and then exploiting Eq.(13) one gets the effective pure state of the two-spin system as follows

$$\begin{aligned} \rho_{eff} &= 2D_0 = \frac{1}{2}E + 2I_{1z}I_{2z} \\ & - \exp(-i\frac{\pi}{2}I_{1x})WDW \exp(i\frac{\pi}{2}I_{1x})(2I_{1z}I_{2z}) \exp(-i\frac{\pi}{2}I_{1x})WDW \exp(i\frac{\pi}{2}I_{1x}) \\ & - \exp(-i\frac{\pi}{2}I_{2x})WDW \exp(i\frac{\pi}{2}I_{2x})(2I_{1z}I_{2z}) \exp(-i\frac{\pi}{2}I_{2x})WDW \exp(i\frac{\pi}{2}I_{2x}) \end{aligned}$$

In NMR experiments of ensemble quantum computation the starting reduced density operator $\sigma(0) = 2I_{1z}I_{2z}$ is first prepared from the equilibrium state in the coupled two-spin ($I=1/2$) system. By starting from the density operator $\sigma(0) = 2I_{1z}I_{2z}$, one performs three different experiments to create three different mixed states, one experiment with identity transformation E and the other two with the unitary transformations: $\exp(-i\frac{\pi}{2}I_{1x})WDW \exp(i\frac{\pi}{2}I_{1x})$ and $\exp(-i\frac{\pi}{2}I_{2x})WDW \exp(i\frac{\pi}{2}I_{2x})$, respectively. Then the created state $\sigma(0) = 2I_{1z}I_{2z}$ minus the other two created states will give the effective pure state $2D_0 - \frac{1}{2}E$.

(b) A three-spin system

The density operator $\sigma_+(0)$ is chosen as $\sigma_+(0) = 4I_{1y}I_{2z}I_{3z}, 4I_{1z}I_{2y}I_{3z}, 4I_{1z}I_{2z}I_{3y}$, and $4I_{1y}I_{2y}I_{3y}$, respectively. With the help of Eq.(14) it easily turns out for the density operator $\sigma_+(0) = 4I_{ky}I_{lz}I_{mz}$ (cyclicly permuting k, l, m) that

$$\begin{aligned} & \frac{2}{N} \exp(-i\frac{\pi}{2}I_{kx})[4I_{ky}I_{lz}I_{mz}, ND_0]_+ \exp(i\frac{\pi}{2}I_{kx}) \\ &= \frac{2}{N} \left\{ \frac{1}{2}(E_k + 2I_{kz}) \otimes (E_l + 2I_{lz}) \otimes (E_m + 2I_{mz}) \right. \\ & \quad \left. - \frac{1}{2}(E_k - 2I_{kz}) \otimes (E_l + 2I_{lz}) \otimes (E_m + 2I_{mz}) \right\} \\ &= 4I_{kz}I_{lz}I_{mz} - \exp(-i\frac{\pi}{2}I_{kx})WDW \exp(i\frac{\pi}{2}I_{kx}) \\ & \quad \times (4I_{kz}I_{lz}I_{mz}) \exp(-i\frac{\pi}{2}I_{kx})WDW \exp(i\frac{\pi}{2}I_{kx}) \end{aligned} \quad (21a)$$

and for the density operator $\sigma_+(0) = 4I_{ky}I_{ly}I_{my}$ that

$$\begin{aligned} & \frac{2}{N} \exp(-i\frac{\pi}{4} \times 8I_{kx}I_{lx}I_{mx})[4I_{ky}I_{ly}I_{my}, ND_0]_+ \exp(i\frac{\pi}{4} \times 8I_{kx}I_{lx}I_{mx}) \\ &= \frac{2}{N} \left\{ -\frac{1}{2}(E_k + 2I_{kz}) \otimes (E_l + 2I_{lz}) \otimes (E_m + 2I_{mz}) \right. \end{aligned}$$

$$\begin{aligned}
& +\frac{1}{2}(E_k - 2I_{kz}) \otimes (E_l - 2I_{lz}) \otimes (E_m - 2I_{mz})\} \\
& = -4I_{kz}I_{lz}I_{mz} \\
& - \exp(-i\frac{\pi}{4} \times 8I_{kx}I_{lx}I_{mx})WDW \exp(i\frac{\pi}{2}F_x) \\
& \times (4I_{kz}I_{lz}I_{mz}) \exp(-i\frac{\pi}{2}F_x)WDW \exp(i\frac{\pi}{4} \times 8I_{kx}I_{lx}I_{mx}) \quad (21b)
\end{aligned}$$

where $F_x = I_{kx} + I_{lx} + I_{mx}$ and $N = 2^3$. Then exploiting Eqs.(21) the effective pure state in the three-spin system can be built up as follows

$$\begin{aligned}
\rho_{eff} & = 2^2 D_0 = \frac{1}{2}E + (2^2 - 1)2^2 I_{1z}I_{2z}I_{3z} \\
& - \sum_{k=1}^3 \{ \exp(-i\frac{\pi}{2}I_{kx})WDW \exp(i\frac{\pi}{2}I_{kx}) \\
& \quad \times (2^2 I_{1z}I_{2z}I_{3z}) \exp(-i\frac{\pi}{2}I_{kx})WDW \exp(i\frac{\pi}{2}I_{kx}) \} \\
& - \exp(-i\frac{\pi}{4} \times 8I_{1x}I_{2x}I_{3x})WDW \exp(-i\frac{\pi}{2}F_x) \\
& \quad \times (2^2 I_{1z}I_{2z}I_{3z}) \exp(i\frac{\pi}{2}F_x)WDW \exp(i\frac{\pi}{4} \times 8I_{1x}I_{2x}I_{3x}).
\end{aligned}$$

Experimentally, one first prepares the starting reduced density operator $\sigma(0) = 4I_{1z}I_{2z}I_{3z}$ from the equilibrium magnetization in a coupled three-spin system. Then only five different experiments are performed in order to prepare the effective pure state $(2^2 D_0 - \frac{1}{2}E)$. If the experimental signal-to-noise ratio is high enough in the spin system the contribution of component $(2^2 - 1)2^2 I_{1z}I_{2z}I_{3z}$ to the effective pure state can be obtained directly by amplifying the amplitude of the longitudinal three-spin order component $2^2 I_{1z}I_{2z}I_{3z}$.

(c) A four-spin system

The density operator $\sigma_+(0)$ is chosen as $\sigma_+(0) = 8I_{1y}I_{2z}I_{3z}I_{4z}$, $8I_{1z}I_{2y}I_{3z}I_{4z}$, $8I_{1z}I_{2z}I_{3y}I_{4z}$, $8I_{1z}I_{2z}I_{3z}I_{4y}$, and $8I_{1z}I_{2y}I_{3y}I_{4y}$, $8I_{1y}I_{2z}I_{3y}I_{4y}$, $8I_{1y}I_{2y}I_{3z}I_{4y}$, $8I_{1y}I_{2y}I_{3y}I_{4z}$, respectively. Then the effective pure state can be easily constructed from Eq.(13) with the help of Eq.(14)

$$\begin{aligned}
\rho_{eff} & = 2^3 D_0 = \frac{1}{2}E + (2^3 - 1) \times 2^3 I_{1z}I_{2z}I_{3z}I_{4z} \\
& - \sum_{k=1}^4 \{ \exp(-i\frac{\pi}{2}I_{kx})WDW \exp(i\frac{\pi}{2}I_{kx}) \\
& \quad \times (8I_{1z}I_{2z}I_{3z}I_{4z}) \exp(-i\frac{\pi}{2}I_{kx})WDW \exp(i\frac{\pi}{2}I_{kx}) \} \\
& - \sum_{m>l>k=1}^4 \{ \exp(-i\frac{\pi}{4} \times 8I_{kx}I_{lx}I_{mx})WDW \exp[-i\frac{\pi}{2}(I_{kx} + I_{lx} + I_{mx})] \\
& \quad \times (8I_{1z}I_{2z}I_{3z}I_{4z}) \exp[i\frac{\pi}{2}(I_{kx} + I_{lx} + I_{mx})]WDW \exp(i\frac{\pi}{4} \times 8I_{kx}I_{lx}I_{mx}) \}
\end{aligned}$$

Obviously, to prepare experimentally the effective pure state $2^3 D_0 - \frac{1}{2}E$ in the four-spin system one needs to perform nine different experiments directly by starting from the density operator $\sigma(0) = 8I_{1z}I_{2z}I_{3z}I_{4z}$.

(d) A five-spin system

The density operator $\sigma_+(0)$ is chosen as $\sigma_+(0) = 2^4 I_{1y}I_{2z}I_{3z}I_{4z}I_{5z}$,

$2^4 I_{1z} I_{2y} I_{3z} I_{4z} I_{5z}, \dots, 2^4 I_{1z} I_{2z} I_{3z} I_{4z} I_{5y}; 2^4 I_{1y} I_{2y} I_{3y} I_{4z} I_{5z}, \dots, 2^4 I_{1z} I_{2z} I_{3y} I_{4y} I_{5y};$
 $2^4 I_{1y} I_{2y} I_{3y} I_{4y} I_{5y}$, respectively. On the basis of Eqs.(13) and (14) the effective pure state can be readily written as

$$\begin{aligned} \rho_{eff} = & 2^4 D_0 = \frac{1}{2} E + (2^4 - 1) \times 2^4 I_{1z} I_{2z} I_{3z} I_{4z} I_{5z} \\ & - \sum_{k=1}^5 \{ \exp(-i \frac{\pi}{2} I_{kx}) W D W \exp(i \frac{\pi}{2} I_{kx}) \\ & \quad \times (2^4 I_{1z} I_{2z} I_{3z} I_{4z} I_{5z}) \exp(-i \frac{\pi}{2} I_{kx}) W D W \exp(i \frac{\pi}{2} I_{kx}) \} \\ & - \sum_{m>l>k=1}^5 \{ \exp(-i \frac{\pi}{4} \times 8 I_{kx} I_{lx} I_{mx}) W D W \exp[-i \frac{\pi}{2} (I_{kx} + I_{lx} + I_{mx})] \\ & \quad \times (2^4 I_{1z} I_{2z} I_{3z} I_{4z} I_{5z}) \exp[i \frac{\pi}{2} (I_{kx} + I_{lx} + I_{mx})] W D W \exp(i \frac{\pi}{4} \times 8 I_{kx} I_{lx} I_{mx}) \} \\ & - \exp(-i \frac{\pi}{4} \times 32 I_{1x} I_{2x} I_{3x} I_{4x} I_{5x}) W D W \exp(i \frac{\pi}{2} F_x) \\ & \quad \times (2^4 I_{1z} I_{2z} I_{3z} I_{4z} I_{5z}) \exp(-i \frac{\pi}{2} F_x) W D W \exp(i \frac{\pi}{4} \times 32 I_{1x} I_{2x} I_{3x} I_{4x} I_{5x}) \end{aligned}$$

This shows that the effective pure state $2^4 D_0 - \frac{1}{2} E$ can be prepared by performing $(2^{5-1} + 1)$ different experiments in the five-spin system.

(e) An arbitrary n-spin ($n \geq 6$) system

The density operator $\sigma_+(0)$ is chosen as $\sigma_+(0) = 2^{n-1} I_{1y} I_{2z} \dots I_{nz}$,
 $2^{n-1} I_{1z} I_{2y} I_{3z} \dots I_{nz}$, ..., $2^{n-1} I_{1z} \dots I_{n-1z} I_{ny}$; $2^{n-1} I_{1y} I_{2y} I_{3y} I_{4z} \dots I_{nz}$, ...,
 $2^{n-1} I_{1z} \dots I_{n-3z} I_{n-2y} I_{n-1y} I_{ny}$; $2^{n-1} I_{1y} I_{2y} I_{3y} I_{4y} I_{5y} I_{6z} \dots I_{nz}$, ...,
 $2^{n-1} I_{1z} \dots I_{n-5z} I_{n-4y} I_{n-3y} I_{n-2y} I_{n-1y} I_{ny}$; , respectively. With the aid of
Eqs.(13) and (14) the effective pure state can be written generally and conveniently as

$$\begin{aligned} \rho_{eff} = & 2^{n-1} D_0 = \frac{1}{2} E + (2^{n-1} - 1) \times 2^{n-1} I_{1z} I_{2z} \dots I_{nz} \\ & - \sum_{k=1}^n \{ \exp(-i \frac{\pi}{2} I_{kx}) W D W \exp(i \frac{\pi}{2} I_{kx}) \\ & \quad \times (2^{n-1} I_{1z} I_{2z} \dots I_{nz}) \exp(-i \frac{\pi}{2} I_{kx}) W D W \exp(i \frac{\pi}{2} I_{kx}) \} \\ & - \sum_{m>l>k=1}^n \{ \exp(-i \frac{\pi}{4} \times 2^3 I_{kx} I_{lx} I_{mx}) W D W \exp[-i \frac{\pi}{2} (I_{kx} + I_{lx} + I_{mx})] \\ & \quad \times (2^{n-1} I_{1z} I_{2z} \dots I_{nz}) \exp[i \frac{\pi}{2} (I_{kx} + I_{lx} + I_{mx})] W D W \exp(i \frac{\pi}{4} \times 2^3 I_{kx} I_{lx} I_{mx}) \} \\ & - \sum_{q>p>m>l>k=1}^n \{ \exp(-i \frac{\pi}{4} \times 2^5 I_{kx} I_{lx} I_{mx} I_{px} I_{qx}) W D W \\ & \quad \times \exp[i \frac{\pi}{2} (I_{kx} + I_{lx} + I_{mx} + I_{px} + I_{qx})] (2^{n-1} I_{1z} I_{2z} \dots I_{nz}) \\ & \quad \times \exp[-i \frac{\pi}{2} (I_{kx} + I_{lx} + I_{mx} + I_{px} + I_{qx})] W D W \exp(i \frac{\pi}{4} \times 2^5 I_{kx} I_{lx} I_{mx} I_{px} I_{qx}) \} \\ & - \dots \end{aligned}$$

It follows from the above expression that one may need to perform $(2^{n-1} + 1)$ different experiments by starting from the density operator, i.e., the longitudinal n -spin order component $\sigma(0) = 2^{n-1} I_{1z} I_{2z} \dots I_{nz}$ in order to prepare experimentally the effective pure state $2^{n-1} D_0 - \frac{1}{2} E$ with n qubits. This

shows that the experiment number to prepare the n -qubit effective pure state by the present method is about half number $(2^n - 1)$ required by the exhaustive averaging method in Ref.[23].

3. Discussion

It has been shown that the effective pure state can be prepared conveniently on the basis of Eq.(13) when the starting reduced density operator is chosen suitably. Experimentally, the effective pure state is prepared generally from the starting density operator, that is, the longitudinal n -spin order component, $\sigma(0) = 2^{n-1} I_{1z} I_{2z} \dots I_{nz}$ in a unified and systematical form, while the latter can be obtained conveniently from the equilibrium magnetization in a coupled n -spin ($I=1/2$) system. Actually, the starting density operator $\sigma(0) = 2^{n-1} I_{1z} I_{2z} \dots I_{nz}$ can be obtained easily from the equilibrium magnetization $\sigma_{keq} \propto I_{kz}$ of any k th spin in the coupled spin ($I=1/2$) system by performing a sequence of one-qubit quantum gate operations and the two-qubit diagonal gate operations $G_{kl}(\lambda_{kl}) = \exp(-i\lambda_{kl} 2I_{kz} I_{lz})$ [26], for example,

$$\begin{aligned} \sigma_{1eq} \propto I_{1z} \frac{\pi I_{1y} I_{2z}}{2} 2 I_{1x} I_{2z} \frac{-\frac{\pi}{2} I_{1y}}{2} 2 I_{1z} I_{2z} \frac{\pi I_{2y} I_{3z}}{2} \frac{-\frac{\pi}{2} I_{2y}}{2} 4 I_{1z} I_{2z} I_{3z} \dots \\ \dots 2^{n-2} I_{1z} I_{2z} \dots I_{n-1z} \frac{\pi I_{n-1y} I_{nz}}{2} \frac{-\frac{\pi}{2} I_{n-1y}}{2} 2^{n-1} I_{1z} I_{2z} \dots I_{nz} = \sigma(0), \end{aligned}$$

where the unitary transformation $\exp(-i\theta P) A \exp(i\theta P) = B$ is denoted briefly as $A \xrightarrow{\theta P} B$. In the high-temperature approximation the thermal equilibrium state of an n -spin system can be written as $\sigma_{eq} \propto \sum_k I_{kz}$. Then $\sigma_{keq} \propto I_{kz}$ can be obtained by first applying a selective 90_x° pulse only to the spin k , then a hard 90_{-x}° pulse to all the spins of the system, and then applying a magnetic field gradient to the system to cancel all the transverse magnetizations I_{ly} ($l \neq k$). The equilibrium magnetization of any one of the spins in the spin system, e.g., the k th spin, usually can be enhanced easily by various polarization transfer processes [11, 24, 25]. Then the present method is a simple scheme to make use of various polarization transfer techniques to scale up the qubit size on an NMR quantum computer [11, 21]. Because the equilibrium magnetization is inverse proportional to the exponential factor 2^n when the high-temperature approximation holds in the coupled n -spin system it is easy to find that the effective pure state prepared by the method has a signal-to-noise ratio inverse proportional to the factor 2^n in each experiment on average, and it is well-known that this

is a general disadvantage of ensemble quantum computation [11, 12, 23]. The present preparation of the effective pure state involves the unitary operations including the n -qubit Walsh-Hadamard transform W , the n -qubit diffusion transform D [5], and the m -body ($1 \leq m \leq n$) elementary propagators $\exp(\pm i\theta 2^{m-1} I_{k_1 x} I_{k_2 x} \dots I_{k_m x})$ built up with the m -body interaction $2^{m-1} I_{k_1 x} I_{k_2 x} \dots I_{k_m x}$ ($1 \leq k_i \leq n$, and $i = 1, 2, \dots, m$) [26, 27]. Each of all these unitary operations is readily decomposed completely into a sequence of one-qubit quantum gates and the two-qubit diagonal quantum gates [26]. Therefore, the present method to prepare the effective pure states could be programmed and performed conveniently on an NMR quantum computer.

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